09393577

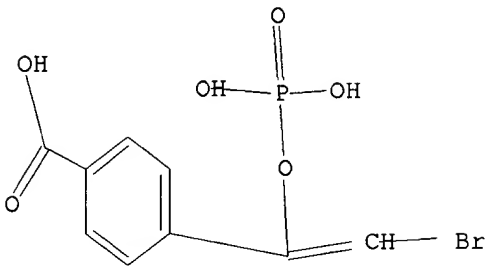
(FILE 'HOME' ENTERED AT 09:55:02 ON 04 SEP 2003)

FILE 'REGISTRY' ENTERED AT 09:55:12 ON 04 SEP 2003

L1 STRUCTURE UPLOADED

L2 0 S L1 SSS FULL

=> d l1
L1 HAS NO ANSWERS
L1 STR

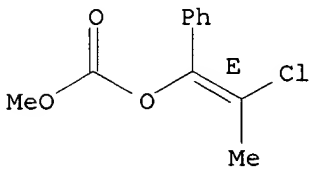


G1 Cb,Cy,Ak

Structure attributes must be viewed using STN Express query preparation.

L7 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2002 ACS
RN **136454-49-4** REGISTRY
CN Carbonic acid, 2-chloro-1-phenyl-1-propenyl methyl ester, (E)- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C11 H11 Cl O3
SR CA
LC STN Files: BEILSTEIN*, CA, CAPLUS, CASREACT
(*File contains numerically searchable property data)

Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

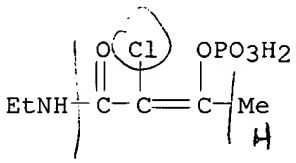
1 REFERENCES IN FILE CA (1962 TO DATE)
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

102

L2 ANSWER 1 OF 1 CAOLD COPYRIGHT 2002 ACS
AN CA57:7553i CAOLD
TI toxicology and pharmacology of a systemic phosphoric acid ester insecticide phosphamidon
AU Jaques, Roland; Bein, H. J.
IT 15844-87-8 **89490-23-3**

=> d l1 all
YOU HAVE REQUESTED DATA FROM FILE 'REGISTRY' - CONTINUE? (Y)/N:y

L1 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2002 ACS
RN **89490-23-3** REGISTRY
CN Crotonamide, 2-chloro-N-ethyl-3-hydroxy-, phosphate (7CI) (CA INDEX NAME)
FS 3D CONCORD
MF C6 H11 Cl N O5 P
LC STN Files: CAOLD



caba - Phosphate

Calculated Properties (CALC)

PROPERTY (CODE)	VALUE	CONDITION	NOTE
Freely Rotatable Bonds (FRB)	7		(1) ACD
H acceptors (HAC)	6		(1) ACD
H donors (HD)	3		(1) ACD
logD (LOGD)	-1.15	pH 1	(1) ACD
logD (LOGD)	-3.65	pH 4	(1) ACD
logD (LOGD)	-5.87	pH 7	(1) ACD
logD (LOGD)	-5.97	pH 8	(1) ACD
logD (LOGD)	-5.99	pH 10	(1) ACD
logP (LOGP)	-0.981+/-0.635		(1) ACD
Molar Solubility (SLB.MOL)	>=0.1 - <1 mol/L	pH 1	(1) ACD
Molar Solubility (SLB.MOL)	>=1 mol/L	pH 4	(1) ACD
Molar Solubility (SLB.MOL)	>=1 mol/L	pH 7	(1) ACD
Molar Solubility (SLB.MOL)	>=1 mol/L	pH 8	(1) ACD
Molar Solubility (SLB.MOL)	>=1 mol/L	pH 10	(1) ACD
Molecular Weight (MW)	243.58		(1) ACD
pKa (PKA)	1.32+/-0.10	Most Acidic	(1) ACD

(1) Calculated using Advanced Chemistry Development (ACD) Software Solaris V4.76 ((C) 1994-2002 ACD)

1 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

L2 ANSWER 1 OF 1 CAOLD COPYRIGHT 2002 ACS
AN CA57:7553i CAOLD
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MF C6 H11 Cl N O5 P
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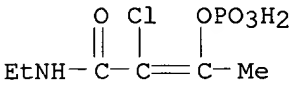

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(1) Calculated using Advanced Chemistry Development (ACD) Software Solaris V4.76 ((C) 1994-2002 ACD)

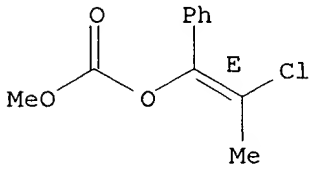
1 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

L9 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2002 ACS
AN 1991:631804 CAPLUS
DN 115:231804
TI Reactions of polyhalo compounds with metals and electrophilic reagents. XII. Reactions of geminal .alpha.,.alpha.-dichloro-, .alpha.,.alpha.-dibromo-, and .alpha.,.alpha.-bromochloro-substituted ketones with zinc and acid chlorides
AU Shchepin, V. V.; Gladkova, G. E.; Neifel'd, P. G.
CS Perm. Gos. Univ., Perm, USSR
SO Zhurnal Organicheskoi Khimii (1990), 26(11), 2394-7
CODEN: ZORKAE; ISSN: 0514-7492
DT Journal
LA Russian
CC 25-18 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)
OS CASREACT 115:231804
AB RCX2COPh (R = Me, Et; X = Cl, Br) reacted with Zn and R1COCl (R1 = Me, Pr, Bu, Me3C, PhCH2, p-tolyl, MeO, p-ClC6H4OCH2) in EtOAc at 40-45.degree. to give 18 corresponding RCX:CPhO2CR1 (I) as mixts. of E and Z isomers, with the former predominating, in 41-83% combined yield. EtCClBr2COPh reacted under these conditions only at the C-Br bond, giving 61-69% I (R = Et, X = Cl; R1 = Et, Pr, CMe3).
ST halo ketone reaction zinc acid chloride; ketone dihalo reaction zinc acid chloride; halophenylalkenyl ester; alkenyl ester halophenyl
IT Carboxylic acids, esters
RL: SPN (Synthetic preparation); PREP (Preparation)
(halophenylalkenyl esters, prepn. of, by reaction of dihaloalkyl Ph ketones with zinc and acid chlorides)
IT Acid chlorides
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with zinc and dihaloalkyl Ph ketones, halophenylalkenyl esters by)
IT Ketones, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(haloalkyl Ph, reaction of, with zinc and acid chlorides, halophenylalkenyl esters by)
IT 54034-55-8P 54034-59-2P 73496-68-1P 136454-29-0P 136454-30-3P
136454-31-4P **136454-32-5P** 136454-33-6P 136454-34-7P
136454-35-8P 136454-36-9P 136454-37-0P 136454-38-1P 136454-39-2P
136454-40-5P 136454-41-6P 136454-42-7P 136454-43-8P 136454-44-9P
136454-45-0P 136454-46-1P 136454-47-2P 136454-48-3P
136454-49-4P 136454-50-7P 136454-51-8P 136454-52-9P
136454-53-0P 136454-54-1P 136454-55-2P 136454-56-3P 136454-57-4P
136454-58-5P 136454-59-6P 136480-44-9P 136509-08-5P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
IT 2114-03-6 57169-51-4 66255-85-4 66498-51-9 137853-30-6
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with zinc and acid chlorides, halophenylalkenyl ester by)
IT 75-36-5, Acetyl chloride 79-22-1, Methyl chlorocarbonate 103-80-0, Phenylacetyl chloride 141-75-3, Butanoyl chloride 638-29-9, Pentanoyl chloride 874-60-2, p-Toluoyl chloride 3282-30-2, Pivaloyl chloride 4122-68-3, (4-Chlorophenoxy)acetyl chloride
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with zinc and dihaloalkyl Ph ketones, halophenylalkenyl esters by)

=>

L7 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2002 ACS
RN **136454-49-4** REGISTRY
CN Carbonic acid, 2-chloro-1-phenyl-1-propenyl methyl ester, (E)- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C11 H11 Cl O3
SR CA
LC STN Files: BEILSTEIN*, CA, CAPLUS, CASREACT
(*File contains numerically searchable property data)

Double bond geometry as shown.



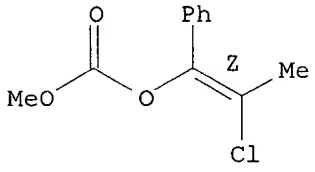
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1962 TO DATE)
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

=>

L8 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2002 ACS
RN **136454-32-5** REGISTRY
CN Carbonic acid, 2-chloro-1-phenyl-1-propenyl methyl ester, (Z)- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C11 H11 Cl O3
SR CA
LC STN Files: BEILSTEIN*, CA, CAPLUS, CASREACT
(*File contains numerically searchable property data)

Double bond geometry as shown.



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IT 15844-87-8 **89490-23-3**

=> d l1 all
YOU HAVE REQUESTED DATA FROM FILE 'REGISTRY' - CONTINUE? (Y)/N:y

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RN **89490-23-3** REGISTRY
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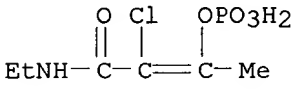
FS 3D CONCORD
MF C6 H11 Cl N O5 P
LC STN Files: CAOLD



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FS STEREOSEARCH
MF C11 H11 Cl O3
SR CA
LC STN Files: BEILSTEIN*, CA, CAPLUS, CASREACT
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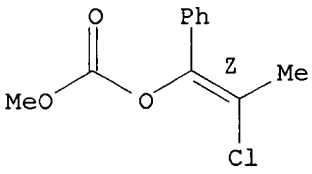

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1 REFERENCES IN FILE CAPLUS (1962 TO DATE)